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Calculation of the radiation trapping force for laser tweezers by use of generalized Lorenz–Mie theory.

I. Localized model description of an on-axis tightly focused laser beam with spherical aberration

James A. Lock

Calculation of the radiation trapping force in laser tweezers by use of generalized Lorenz–Mie theory requires knowledge of the shape coefficients of the incident laser beam. The localized version of these coefficients has been developed and justified only for a moderately focused Gaussian beam polarized in the x direction and traveling in the positive z direction. Here the localized model is extended to a beam tightly focused and truncated by a high-numerical-aperture lens, aberrated by its transmission through the wall of the sample cell, and incident upon a spherical particle whose center is on the beam axis. We also consider polarization of the beam in the y direction and propagation in the negative z direction to be able to describe circularly polarized beams and reflected beams. © 2004 Optical Society of America
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1. Introduction

In the years since their invention in 1986 by Ashkin and his coworkers,¹ laser tweezers have enjoyed a wide range of applications when small biological structures or other small particles are to be noninvasively held and manipulated. It may be argued that the predictive power of the theory of laser tweezers has lagged somewhat behind experimental progress. For example, relatively little theoretical progress has been made on calculating the radiation force and torque on a nonspherical particle (see, however, Ref. 2). For a spherical particle there appears at present to be no single practical theory that is equally applicable to particles of all sizes and to all laser beam profiles. Nonetheless, reasonable agreement between theory and experiment has been achieved^{3,4} for both very small and very large particles for which wave scattering theory simplifies to Rayleigh scattering or geometrical optics, respectively. If the spherical particle being held by the

laser beam is in the Rayleigh scattering regime, the radiation trapping force is accurately calculated by use of the gradient-plus-scattering-force model.^{1,5–10} This model assumes that the trapping laser beam is either a freely diffracting focused Gaussian laser beam^{5–7} or, more realistically, a Gaussian laser beam that (i) is truncated and focused by a high-numerical-aperture (NA) oil-immersion microscope objective lens and (ii) possesses spherical aberration owing to its transmission from the microscope coverslip to the liquid-filled sample cell.^{8–10} At the other end of the particle size spectrum, geometrical ray optics has been relatively successful compared with the appropriate experiments.^{11–15} Ray models have the drawbacks that the interaction of the beam with the particle being trapped sums the various physical scattering processes such as reflection, transmission, and transmission following a number of internal reflections incoherently rather than coherently and that it models the trapping beam as a truncated and perfectly focused ray bundle rather than as the aberrated beam encountered in experiments.

In principle, generalized Lorenz–Mie scattering theory (GLMT) applied to the radiation trapping force should be able to bridge the gap between the Rayleigh and ray scattering regimes. But, for the most part, a simple and efficient GLMT scattering calculation of the trapping force has not been developed. Though the Mie theory formula for the trap-

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ping force has been known for two decades,^{16–18} it possesses the inconvenience that the trapping beam must be expressed in terms of an infinite series of transverse electric (TE) and transverse magnetic (TM) spherical multipole waves. These waves are multiplied by a set of TE and TM coefficients, known as the beam shape coefficients, which give the amplitude and the phase of each spherical multipole wave in the expansion of the beam. In principle, each beam shape coefficient can be computed as an angular integral of the radial component of the beam's electric or magnetic field multiplied by the complex conjugate of the appropriate spherical multipole field.^{17,19,20} But, if many such coefficients are required for the computation of the trapping force, as is the case when the size of the trapped particle is comparable to or larger than the laser wavelength, the evaluation of these coefficients becomes laborious. As an alternative, the shape coefficients of a focused Gaussian beam propagating in the positive z direction whose electric field is polarized in the x direction when the center of the particle being trapped lies on the beam axis²¹ have been determined in a simple way by use of an extension of van de Hulst's localization principle.²² This localized model of an x -polarized Gaussian beam has been extended to the case when the center of the particle that is being trapped does not lie on the beam axis.²³ To date, the localized beam model has been extensively tested only for a moderately focused Gaussian beam,^{24–28} and only a small number of specialized GLMT radiation trapping force calculations that use the localized beam model have been reported.^{29–32}

Before radiation trapping calculations can be done, the incident beam must be accurately modeled. The subject of this paper is the extension of the localized beam model in the context of GLMT to the tightly focused, truncated, and aberrated beams used in laser tweezer experiments. In a companion paper³³ this extension of the localized beam model is used to calculate the trapping force on a spherical particle whose size can range from the Rayleigh scattering limit to the ray theory limit, and the results are compared with the experiments of Refs. 4 and 34.

I intend to examine the extension of the GLMT method to trapping by off-axis beams in a future paper. The reader interested primarily in the operation of laser tweezers rather than in the specific electromagnetic details of localized-model beams may finish this section, read Section 2 to become familiar with the notation used here, and then proceed to the conclusions summarized in Section 6. In the research reported in Ref. 33 it was found that GLMT accompanied by the localized model of the trapping laser beam provides a promising candidate for calculating the radiation trapping force of any profile laser beam on any size spherical particle in a practical way. GLMT calculations produce the experimentally observed decrease in trapping efficiency as the particle is located deeper in the sample cell. But all the effort made here to carefully model a realistic beam in laser tweezer experiments appears to give only a

small change in the calculated trapping efficiency from that which uses the theoretically much simpler but experimentally unrealistic focused Gaussian beam model. As a result, any difference between the experimental and the calculated trapping efficiencies would appear to be due to effects other than electromagnetic beam modeling.

The body of this paper is organized as follows: In Section 2, I carry out the decomposition of a beam linearly polarized in either the x or the y direction, traveling in either the positive or the negative z direction, and with the center of the particle trapped on the z axis, in terms of an infinite series of spherical multipole waves multiplied by beam shape coefficients. The basic properties of the beam shape coefficients are also discussed. Both x and y linearly polarized beams are described, so two such beams 90° out of phase may be superposed to produce a circularly polarized beam, which is necessary for the production of an optical torque on a particle.^{35,36} I expect to address the calculation of optical torques by use of the GLMT in a future paper. In Section 3, I briefly summarize the formulas for both a freely diffracting focused Gaussian beam and a plane wave truncated and focused by a high-NA lens and then either reflected or refracted by a flat interface located before the beam's focal waist. The field components of these beams are expressed as analytic functions or integrals over analytic functions rather than in terms of spherical multipole waves. In Section 4, I extend the procedure for determining the localized beam shape coefficients to an arbitrary beam polarized in either the x or the y direction and propagating in either the z or the $-z$ direction, as long as the center of the particle being trapped lies on the beam axis, and apply the procedure to the Gaussian beam and the truncated, focused, and aberrated beam of Section 3. In Section 5, I numerically reconstruct a tightly focused localized Gaussian beam and a truncated, tightly focused, and aberrated localized beam from the spherical multiple waves and beam shape coefficients and compare the result with the properties of the original beams of Section 3 from which the localized shape coefficients were obtained. Lastly, in Section 6 I state my conclusions concerning the applicability of the localized beam model to a tightly focused beam. In each section of this paper new results are presented along with results that were published before. The earlier results are suitably referenced.

2. Expansion of an On-Axis Beam in Terms of Spherical Multipole Waves

Consider an electromagnetic beam of frequency ω , free-space wavelength λ , free-space wave number $k = 2\pi/\lambda$, field strength E_0 , time dependence $\exp(-i\omega t)$, and propagating in a medium of refractive index n , that is an exact solution to Maxwell's equations. According to electromagnetic theory, the electric and magnetic fields of the beam may be expressed in spherical coordinates as an infinite series of TE and TM spherical multipole waves of partial wave num-

ber l and azimuthal mode number m . In the notation of Refs. 20 and 24, the fields are

$$\mathbf{E} = E_0(e_r \mathbf{u}_r + e_\theta \mathbf{u}_\theta + e_\phi \mathbf{u}_\phi), \quad (1a)$$

$$\mathbf{B} = (nE_0/c)(b_r \mathbf{u}_r + b_\theta \mathbf{u}_\theta + b_\phi \mathbf{u}_\phi), \quad (1b)$$

where c is the speed of light in vacuum and^{17,19}

$$e_r(r, \theta, \phi) = -i \sum_{l=1}^{\infty} \sum_{m=-l}^l l(l+1) A_{l,m} [j_l(nkr)/(nkr)] \times \pi_l^{|m|}(\theta) \sin(\theta) \exp(im\phi), \quad (2a)$$

$$e_\theta(r, \theta, \phi) = i \sum_{l=1}^{\infty} \sum_{m=-l}^l [m B_{l,m} j_l(nkr) \pi_l^{|m|}(\theta) - A_{l,m} L_l(nkr) \tau_l^{|m|}(\theta)] \exp(im\phi), \quad (2b)$$

$$e_\phi(r, \theta, \phi) = - \sum_{l=1}^{\infty} \sum_{m=-l}^l [B_{l,m} j_l(nkr) \tau_l^{|m|}(\theta) - m A_{l,m} L_l(nkr) \pi_l^{|m|}(\theta)] \exp(im\phi), \quad (2c)$$

$$b_r(r, \theta, \phi) = -i \sum_{l=1}^{\infty} \sum_{m=-l}^l l(l+1) B_{l,m} [j_l(nkr)/(nkr)] \times \pi_l^{|m|}(\theta) \sin(\theta) \exp(im\phi), \quad (2d)$$

$$b_\theta(r, \theta, \phi) = -i \sum_{l=1}^{\infty} \sum_{m=-l}^l [m A_{l,m} j_l(nkr) \pi_l^{|m|}(\theta) + B_{l,m} L_l(nkr) \tau_l^{|m|}(\theta)] \exp(im\phi), \quad (2e)$$

$$b_\phi(r, \theta, \phi) = \sum_{l=1}^{\infty} \sum_{m=-l}^l [A_{l,m} j_l(nkr) \tau_l^{|m|}(\theta) + m B_{l,m} L_l(nkr) \pi_l^{|m|}(\theta)] \exp(im\phi). \quad (2f)$$

In Eqs. (2a)–(2f) the radial and angular functions are

$$L_l(nkr) \equiv j_l(nkr)/(nkr) + j_l'(nkr), \quad (3)$$

$$\pi_l^{|m|}(\theta) \equiv P_l^{|m|}[\cos(\theta)]/\sin(\theta), \quad (4a)$$

$$\tau_l^{|m|}(\theta) \equiv (d/d\theta) P_l^{|m|}[\cos(\theta)], \quad (4b)$$

where $P_l^{|m|}[\cos(\theta)]$ are associated Legendre polynomials as defined in Ref. 37. In Eqs. (2) the spherical Bessel functions $j_l(nkr)$ are appropriate to beam propagation because both the beam fields and the spherical Bessel functions are finite at the origin, whereas spherical Neumann and Hankel functions diverge there. Beam shape coefficients $A_{l,m}$ and $B_{l,m}$ give the amplitude and the phase of the TM and TE spher-

ical multipole components of the beam and are obtained from the beam fields by^{17,19,20}

$$A_{l,m} = (i/2\pi) \{ (2l+1)/[2l(l+1)] \} [(l-|m|)!/(l+|m|)!] [nkr/j_l(nkr)] \int_0^\pi \sin(\theta) d\theta \times \int_0^{2\pi} d\phi e_r(r, \theta, \phi) P_l^{|m|}[\cos(\theta)] \exp(-im\phi), \quad (5a)$$

$$B_{l,m} = (i/2\pi) \{ (2l+1)/[2l(l+1)] \} [(l-|m|)!/(l+|m|)!] [nkr/j_l(nkr)] \int_0^\pi \sin(\theta) d\theta \times \int_0^{2\pi} d\phi b_r(r, \theta, \phi) P_l^{|m|}[\cos(\theta)] \exp(-im\phi). \quad (5b)$$

The factor $(i^l)(2l+1)/[2l(l+1)]$ that appeared explicitly in the formulas for the field components in Refs. 20 and 24 has been absorbed into the beam shape coefficients in Eqs. (2). If e_r and b_r in Eqs. (5) are the radial components of an exact solution of Maxwell's equations, the angular integrals in Eqs. (5) must be proportional to $j_l(nkr)/(nkr)$ to ensure that $A_{l,m}$ and $B_{l,m}$ are constants. Inasmuch as beam field strength E_0 multiplies the dimensionless beam components e_i and b_i for $i = r, \theta, \phi$ in Eqs. (1), the beam shape coefficients depend only on the shape of the beam and not on its amplitude. Equations (2) and (5) may be used in either of two ways. First, if one knows the exact beam fields analytically, the angular integrals in Eqs. (5) may be performed to yield the shape coefficients of the known beam. Alternatively, if one is given a set of shape coefficients, one may use Eqs. (2) to reconstruct the beam fields that correspond to the coefficients. This reconstruction was performed in Refs. 27 and 28 for a focused Gaussian beam and in Ref. 38 for a top-hat beam. In Section 4 below, we are interested primarily in the second point of view.

Consider a spherical particle whose center is at the origin of an xyz rectangular coordinate system. Qualitatively speaking, if a beam incident upon the particle propagates in either the positive or the negative z direction and possesses an axis of symmetry, the beam is termed on axis if its symmetry axis coincides with the z axis and it is termed off axis if the beam symmetry axis is parallel to the z axis. Mathematically, an on-axis beam contains only the azimuthal modes $m = \pm 1$, whereas an off-axis beam contains all azimuthal modes, $-l \leq m \leq l$. For an on-axis beam, if one wishes to reconstruct the beam fields from the beam shape coefficients, the choice of $A_{l,1}$, $A_{l,-1}$, $B_{l,1}$, and $B_{l,-1}$ is not entirely arbitrary.

To ensure that the rectangular coordinate system's field components remain finite everywhere in the xy plane and that the electric and magnetic fields are orthogonal, the beam shape coefficients must satisfy either $A_{l,1} = A_{l,-1}$ and $B_{l,1} = -B_{l,-1}$ or $A_{l,1} = -A_{l,-1}$ and $B_{l,1} = B_{l,-1}$.

There are four general on-axis beam geometries. For the first of these, the beam propagates in the positive z direction and its electric field is linearly polarized in the x direction. The beam shape coefficients are of the form

$$A_{l,\pm 1} = (i^l)(2l+1)g_l/[2l(l+1)], \quad (6a)$$

$$B_{l,\pm 1} = \mp i(i^l)(2l+1)h_l/[2l(l+1)]. \quad (6b)$$

Hereafter g_l and h_l will also be termed the shape coefficients of the on-axis beam. In Ref. 39, only the case $g_l = h_l$ was considered, whereas here the more-general case $g_l \neq h_l$ is examined as well. The term $(i^l)(2l+1)/[2l(l+1)]$ in Eqs. (6) describes the implicit $\exp(inkz)$ dependence of the beam fields. The ϕ dependence of the fields of Eqs. (2) factors out, giving

$$\mathbf{E} = E_0[G_1^e \cos(\phi)\mathbf{u}_r + G_2^e \cos(\phi)\mathbf{u}_\theta - G_3^e \sin(\phi)\mathbf{u}_\phi], \quad (7a)$$

$$\mathbf{B} = (nE_0/c)[G_1^b \sin(\phi)\mathbf{u}_r + G_2^b \sin(\phi)\mathbf{u}_\theta + G_3^b \cos(\phi)\mathbf{u}_\phi], \quad (7b)$$

with

$$G_1^e(r, \theta) = -i \sum_{l=1}^{\infty} i^l(2l+1) \times g_l[j_l(nkr)/(nkr)]\pi_l(\theta)\sin(\theta), \quad (8a)$$

$$G_2^e(r, \theta) = \sum_{l=1}^{\infty} \{i^l(2l+1)/[l(l+1)]\}[h_l j_l(nkr)\pi_l(\theta) - ig_l L_l(nkr)\tau_l(\theta)], \quad (8b)$$

$$G_3^e(r, \theta) = \sum_{l=1}^{\infty} \{i^l(2l+1)/[l(l+1)]\}[h_l j_l(nkr)\tau_l(\theta) - ig_l L_l(nkr)\pi_l(\theta)], \quad (8c)$$

$$G_1^b(r, \theta) = -i \sum_{l=1}^{\infty} i^l(2l+1) \times h_l[j_l(nkr)/(nkr)]\pi_l(\theta)\sin(\theta), \quad (8d)$$

$$G_2^b(r, \theta) = \sum_{l=1}^{\infty} \{i^l(2l+1)/[l(l+1)]\}[g_l j_l(nkr)\pi_l(\theta) - ih_l L_l(nkr)\tau_l(\theta)], \quad (8e)$$

$$G_3^b(r, \theta) = \sum_{l=1}^{\infty} \{i^l(2l+1)/[l(l+1)]\}[g_l j_l(nkr)\tau_l(\theta) - ih_l L_l(nkr)\pi_l(\theta)]; \quad (8f)$$

$$\pi_l(\theta) \equiv \pi_l^1(\theta), \quad (9a)$$

$$\tau_l(\theta) \equiv \tau_l^1(\theta). \quad (9b)$$

If one defines

$$F_1^u \equiv G_1^u \sin(\theta) + G_2^u \cos(\theta), \quad (10a)$$

$$F_2^u \equiv G_1^u \sin(\theta) + G_2^u \cos(\theta) - G_3^u, \quad (10b)$$

$$F_3^u \equiv G_1^u \cos(\theta) - G_2^u \sin(\theta) \quad (10c)$$

for $u = e, b$, the beam fields in rectangular coordinates become

$$\mathbf{E} = E_0\{[F_1^e - F_2^e \sin^2(\phi)]\mathbf{u}_x + F_2^e \sin(\phi)\cos(\phi)\mathbf{u}_y + F_3^e \cos(\phi)\mathbf{u}_z\}, \quad (11a)$$

$$\mathbf{B} = (nE_0/c)\{F_2^b \sin(\phi)\cos(\phi)\mathbf{u}_x + [F_1^b - F_2^b \cos^2(\phi)]\mathbf{u}_y + F_3^b \sin(\phi)\mathbf{u}_z\}. \quad (11b)$$

To make \mathbf{E} and \mathbf{B} appear more symmetric, the fields have sometimes been written⁴⁰ in terms of $\cos(2\phi)$ and $\sin(2\phi)$ rather than in terms of $\cos^2(\phi)$ and $\sin^2(\phi)$.

The three other general on-axis beam geometries and their beam shape coefficients are as follows: If the on-axis beam propagates in the positive z direction and its electric field is linearly polarized in the y direction, the beam shape coefficients are

$$A_{l,\pm 1} = \mp i(i^l)(2l+1)g_l/[2l(l+1)], \quad (12a)$$

$$B_{l,\pm 1} = -(i^l)(2l+1)h_l/[2l(l+1)]. \quad (12b)$$

One then obtains

$$\begin{aligned} \mathbf{E} &= E_0[G_1^e \sin(\phi)\mathbf{u}_r + G_2^e \sin(\phi)\mathbf{u}_\theta + G_3^e \cos(\phi)\mathbf{u}_\phi] \\ &= E_0\{F_2^e \sin(\phi)\cos(\phi)\mathbf{u}_x + [F_1^e - F_2^e \cos^2(\phi)]\mathbf{u}_y + F_3^e \sin(\phi)\mathbf{u}_z\}, \end{aligned} \quad (13a)$$

$$\begin{aligned} \mathbf{B} &= (nE_0/c)[-G_1^b \cos(\phi)\mathbf{u}_r - G_2^b \cos(\phi)\mathbf{u}_\theta + G_3^b \sin(\phi)\mathbf{u}_\phi] \\ &= (nE_0/c)\{-[F_1^b - F_2^b \sin^2(\phi)]\mathbf{u}_x - F_2^b \sin(\phi)\cos(\phi)\mathbf{u}_y - F_3^b \cos(\phi)\mathbf{u}_z\}. \end{aligned} \quad (13b)$$

If the on-axis beam propagates in the $-z$ direction and its electric field is linearly polarized in the x direction, the beam shape coefficients are

$$A_{l,\pm 1} = -(-i)^l(2l+1)g_l/[2l(l+1)], \quad (14a)$$

$$B_{l,\pm 1} = \mp i(-i)^l(2l+1)h_l/[2l(l+1)]. \quad (14b)$$

The term $(-i)^l(2l+1)/[2l(l+1)]$ describes the implicit $\exp(-inkz)$ dependence of the beam fields. One obtains the expressions for G_i^e and G_i^b in this case by taking the complex conjugate of everything in Eqs. (8) with the exception of g_l and h_l . Equations (7a), (10), and (11a) then remain identical, whereas the right-hand sides of Eqs. (7b) and (11b) are multiplied by -1 . Lastly, if the beam propagates in the $-z$ direction and its electric field is linearly polarized in the y direction, the beam shape coefficients are

$$A_{l,\pm 1} = \pm i(-i)^l(2l+1)g_l/[2l(l+1)], \quad (15a)$$

$$B_{l,\pm 1} = -(-i)^l(2l+1)h_l/[2l(l+1)]. \quad (15b)$$

Again, the expressions for G_i^e and G_i^b are identical to those for an x -polarized beam propagating in the $-z$ direction and Eqs. (10) and (13a) remain identical, whereas the right-hand side of Eq. (13b) is multiplied by -1 . For each of the four general on-axis beam geometries, a plane wave is described by $g_l = h_l = 1$.

Two different measures of the beam cross section are useful in calculations of radiation trapping. First, the intensity in the $\pm z$ direction,

$$I_{\pm z} = (\mathbf{E}^* \times \mathbf{B}) \cdot (\pm \mathbf{u}_z) / \mu_0, \quad (16)$$

where μ_0 is the permeability of free space, is used in the calculation of the beam power. Second, the radiation force on a particle in the Rayleigh regime is proportional^{1,5} to the gradient of the quantity $\mathbf{E}^* \cdot \mathbf{E}$. For a beam propagating in the $\pm z$ direction and polarized in the x direction, one obtains

$$I_{\pm z} = (nE_0^2 / \mu_0 c) [F_1^{e*} F_1^b - (F_2^{e*} F_1^b + F_1^{e*} F_2^b) / 2 + \cos(2\phi) (F_2^{e*} F_1^b - F_1^{e*} F_2^b) / 2], \quad (17)$$

$$\mathbf{E}^* \cdot \mathbf{E} = (E_0^2) \{ [F_1^{e*} F_1^e + F_3^{e*} F_3^e + (F_1^{e*} - F_2^{e*}) \times (F_1^e - F_2^e)] / 2 + \cos(2\phi) (F_3^{e*} F_3^e - F_2^{e*} F_2^e + F_1^{e*} F_2^e + F_2^{e*} F_1^e) / 2 \}, \quad (18)$$

whereas for a beam propagating in the $\pm z$ direction and polarized in the y direction the expressions for $I_{\pm z}$ and $\mathbf{E}^* \cdot \mathbf{E}$ are the same as Eqs. (17) and (18), except that $\cos(2\phi)$ is replaced by $-\cos(2\phi)$.

When a high-symmetry beam propagates in a single medium, it appears to be possible to restrict the on-axis beam shape coefficients to $g_l = h_l$ without loss of generality. Such has been found to be the case for a plane wave, a freely diffracting focused Gaussian beam, a Davis first-order focused Gaussian beam,⁴¹ Davis-Barton symmetrized third-order and fifth-order focused Gaussian beams,⁴² and a plane wave focused by a lens.⁴³⁻⁴⁴ In each of these situations one starts with the fact that $F_1^e = F_1^b$ and $F_3^e = F_3^b$. When these equations are substituted into Eqs. (11) and (13) to yield e_r and b_r , and results are then substituted into Eqs. (5), one obtains $g_l = h_l$. The condition $g_l \neq h_l$ arises from symmetry breaking of a $g_l = h_l$ beam, e.g., reflection or refraction of a normally incident beam by a flat interface.^{45,46} In this situation the TE and TM Fresnel coefficients of the associated rays that compose the reflected and refracted beams differ, giving $F_1^e \neq F_1^b$ and $F_3^e \neq F_3^b$, and hence $g_l \neq h_l$. This notation is discussed more fully in Section 3.

3. Field Components of Specific Beams

A. Freely Diffracting Focused Gaussian Beam

An approximation to an on-axis freely diffracting focused Gaussian beam propagating in the z direction and polarized in the x direction is obtained by Fresnel diffracting electric and magnetic fields with flat phase fronts and a Gaussian amplitude profile of half-width w in the $z = z_0$ focal plane:

$$\mathbf{E} = E_0 \exp(-\rho^2/w^2) \mathbf{u}_x, \quad (19a)$$

$$\mathbf{B} = (nE_0/c) \exp(-\rho^2/w^2) \mathbf{u}_y, \quad (19b)$$

where

$$\rho \equiv r \sin(\theta) \quad (20)$$

is the distance of the field point from the z axis to any other parallel plane. The result is

$$F_1^e = F_1^b = D \exp[i\mathbf{k}(z - z_0)] \exp(-D\rho^2/w^2), \quad (21a)$$

$$F_2^e = F_2^b = F_3^e = F_3^b = 0, \quad (21b)$$

where

$$D \equiv [1 + 2is(z - z_0)/w]^{-1}, \quad (22)$$

the beam confinement parameter is

$$s \equiv 1/(nkw), \quad (23)$$

and the field strength at the center of the beam's focal waist is E_0 . This type of beam is produced by focusing an initially Gaussian beam by use of a long-focal-length lens whose aperture is much larger than the beam width such that none of the beam is cut off by the lens. The beam converges to a moderately large focal waist whose center is at the coordinate $z = z_0$ and then reexpands. The $s \rightarrow 0$ limit of Eqs. (21) is a plane wave. The freely diffracting focused Gaussian beam of Eqs. (21) is not an exact solution of Maxwell's equations. However, a procedure was devised by Davis⁴¹ and extended by Barton and Alexander⁴² that obtains a beam in the form of an infinite series in powers of s that both is an exact solution of Maxwell's equations and has Eqs. (21) as its first term. When Eqs. (11) are used to convert from the rectangular components of the fields to the F_i^u functions, the Davis-Barton symmetrized fifth-order beam truncates F_1^e , F_1^b , F_2^e , and F_2^b at $O(s^4)$ and F_3^e , F_3^b at $O(s^5)$, giving

$$F_1^e = F_1^b = D[1 + s^2(3\rho^2 D^2/w^2 - \rho^4 D^3/w^4) + s^4(10\rho^4 D^4/w^4 - 5\rho^6 D^5/w^6 + \rho^8 D^6/2w^8)] \exp[i\mathbf{k}(z - z_0)] \exp(-D\rho^2/w^2), \quad (24a)$$

$$F_2^e = F_2^b = (2\rho^2 D^3/w^2)[s^2 + s^4(4\rho^2 D^2/w^2 - \rho^4 D^3/w^4)] \exp[i\mathbf{k}(z - z_0)] \exp(-D\rho^2/w^2), \quad (24b)$$

$$F_3^e = F_3^b = -(2is\rho D/w) F_1^e. \quad (24c)$$

The Davis first-order beam truncates Eqs. (24) at $O(s^0)$ and $O(s^1)$, and the Davis-Barton symmetrized third-order beam truncates them at $O(s^2)$ and $O(s^3)$. Whereas the entire infinite series in s for the beam is an exact solution of Maxwell's equations, its truncation at first, third, or fifth order is not. The Davis first-order beam description with $s \ll 1$ is a good approximation to the TEM₀₀ mode of a laser beam focused by a long-focal-length lens. But, for a more tightly fo-

cused beam with larger s , the Davis third-order or fifth-order beam description is required for modeling the focused beam more closely, as long as the lens aperture is much larger than the width of the incident beam. For a mildly focused beam F_1^u is dominant and F_2^u and F_3^u are small, where $u = e, b$, because the leading term in F_3^u is proportional to s and the leading term in F_2^u is proportional to s^2 . But, as the beam becomes more tightly focused and s increases, first F_3^u grows in size and becomes comparable to F_1^u and then F_2^u becomes comparable in size as well.

B. Plane Wave Focused by a Lens and Reflected or Refracted by a Plane Interface

The situation is different if the beam is focused by a microscope objective lens whose aperture is smaller than the width of the beam incident upon it, thus cutting off part of the incident beam. Consider a plane wave of electric field strength E_0 traveling in the z direction, linearly polarized in the x direction, and normally incident upon a circularly symmetric aberration-free lens that satisfies the Abbe sine condition and has focal length F , refractive index n_1 , zero absorptivity, and numerical aperture

$$\text{NA} = n_1 \sin(\alpha), \quad (25)$$

where α is the maximum convergence angle of the lens. An expression for the beam fields focused by such a lens was derived in Refs. 43 and 44 by the angular-spectrum-of-plane-waves method. The fields were obtained with the assumption that the beam refracted by the lens is still in the medium of refractive index n_1 , as it is for an oil-immersion microscope objective lens with the beam in the index-matching oil or in the microscope coverslip beneath it. At each point on the lens's input plane, the normally incident electric field vector is decomposed into TE and TM components. Passage of the plane wave through the lens generates a secondary plane wave at each point in the lens's exit plane. The corresponding TE and TM components of the electric field of the secondary plane waves in the angular spectrum of the refracted beam are then recombined to produce the transmitted electric field. The focused beam is polarized in the x direction for $\phi = \pi/2$, in the xz plane for $\phi = 0$, and in a direction containing a y component as well for all other values of ϕ . The fields are then integrated over the lens aperture to give

$$F_i^e = F_i^b = -in_1 k F \int_0^\alpha \sin(\theta_1) d\theta_1 [\cos(\theta_1)]^{1/2} \times \exp[in_1 k(z - z_0) \cos(\theta_1)] p_i, \quad (26)$$

where $i = 1, 2, 3$ and

$$p_1 = (1/2)\{[1 + \cos(\theta_1)]J_0[n_1 k \rho \sin(\theta_1)] + [1 - \cos(\theta_1)]J_2[n_1 k \rho \sin(\theta_1)]\}, \quad (27a)$$

$$p_2 = [1 - \cos(\theta_1)]J_2[n_1 k \rho \sin(\theta_1)], \quad (27b)$$

$$p_3 = -i \sin(\theta_1)J_1[n_1 k \rho \sin(\theta_1)]. \quad (27c)$$

The angle that the propagation direction of a secondary plane wave makes with the z axis is θ_1 , and J_0 , J_1 , and J_2 are Bessel functions that arise from integrating over the azimuthal component of the locations on the lens's exit plane. The center of the resultant beam's focal waist is located at the coordinate $z = z_0$, and the $[\cos(\theta_1)]^{1/2}$ factor is required for satisfying the Abbe sine condition.

C. Example of $g_i \neq h_i$: Plane Wave Focused by a Lens and Reflected or Refracted by a Plane Interface

The beam of Eqs. (26) and (27) is incident upon a flat interface parallel to the xy plane at coordinate $z = d$ with $d < z_0$ separating the medium of refractive index n_1 for $z < d$, such as a microscope coverslip used as the wall of a water-filled sample cell, from another medium that has refractive index n_2 for $z > d$, such as the water in the sample cell. The beams transmitted and reflected by the interface are obtained as follows^{45,46}: For each component plane wave in the angular spectrum of Eqs. (26) and (27), the electric and magnetic fields incident upon the interface are decomposed into TE and TM components. Each component is then multiplied by the respective Fresnel transmission or reflection coefficient, and the TE and TM components in the transmitted or reflected medium are recombined to produce the transmitted or reflected beam. The transmitted fields were derived in Refs. 45 and 46 and are

$$F_i^u = -in_1 k F \int_0^\alpha \sin(\theta_1) d\theta_1 [\cos(\theta_1)]^{1/2} \times \exp\{i[n_2 k \cos(\theta_2)(z - d) - n_1 k \cos(\theta_1)(z_0 - d)]\} p_i^u \quad (28)$$

for $u = e, b$ and $i = 1, 2, 3$, where

$$p_1^e = (1/2)\{[t_{\text{TE}} + t_{\text{TM}} \cos(\theta_2)]J_0[n_1 k \rho \sin(\theta_1)] + [t_{\text{TE}} - t_{\text{TM}} \cos(\theta_2)]J_2[n_1 k \rho \sin(\theta_1)]\}, \quad (29a)$$

$$p_2^e = [t_{\text{TE}} - t_{\text{TM}} \cos(\theta_2)]J_2[n_1 k \rho \sin(\theta_1)], \quad (29b)$$

$$p_3^e = -it_{\text{TM}} \sin(\theta_2)J_1[n_1 k \rho \sin(\theta_1)], \quad (29c)$$

$$p_1^b = (1/2)\{[t_{\text{TM}} + t_{\text{TE}} \cos(\theta_2)]J_0[n_1 k \rho \sin(\theta_1)] + [t_{\text{TM}} - t_{\text{TE}} \cos(\theta_2)]J_2[n_1 k \rho \sin(\theta_1)]\}, \quad (29d)$$

$$p_2^b = [t_{\text{TM}} - t_{\text{TE}} \cos(\theta_2)]J_2[n_1 k \rho \sin(\theta_1)], \quad (29e)$$

$$p_3^b = -it_{\text{TE}} \sin(\theta_2)J_1[n_1 k \rho \sin(\theta_1)]; \quad (29f)$$

$$n_1 \sin(\theta_1) = n_2 \sin(\theta_2). \quad (30)$$

In Eqs. (28) and (29), θ_2 is the refracted angle that a component plane wave makes with the z axis in the medium of refractive index n_2 , and z_0 is the coordi-

nate that the paraxial focal point of the beam would have had if the interface were not present. The electric field Fresnel transmission coefficients are

$$t_{TE} = 2 \cos(\theta_1) / [\cos(\theta_1) + (n_2/n_1)\cos(\theta_2)], \quad (31a)$$

$$t_{TM} = 2 \cos(\theta_1) / [(n_2/n_1)\cos(\theta_1) + \cos(\theta_2)]. \quad (31b)$$

Owing to refraction at the interface, the coordinate of the paraxial focal point of the transmitted beam is now^{45,46}

$$z_{\text{focus}} = z_0 - (n_1 - n_2)(z_0 - d)/n_1. \quad (32)$$

The difference in the amount of refraction experienced by each component plane wave in the angular spectrum at the flat interface causes spherical aberration of the transmitted beam. The spherical aberration caustic in the short-wavelength limit comprises a horn-shaped caustic surrounding an axial spike caustic joined at the paraxial focal point. Near the paraxial focal point the horn caustic is the cusp of revolution whose shape is

$$\rho^2 = 8n_1^3 v^3 / [27n_2(n_1^2 - n_2^2)(z_0 - d)], \quad (33)$$

with

$$v = z_{\text{focus}} - z. \quad (34)$$

This shape is obtained by Taylor-series expansion of the phase of Eq. (28). One should note that the horn-shaped caustic opens toward $-z$ if $n_1 > n_2$ and it opens toward $+z$ if $n_1 < n_2$. Plots of the caustic's diffraction structure are given in Refs. 8 and 47.

By a similar calculation, the fields of the beam reflected by the interface are found to be

$$\begin{aligned} F_i^u = & -in_1 k F \int_0^\alpha \sin(\theta_1) d\theta_1 [\cos(\theta_1)]^{1/2} \\ & \times \exp\{i[-n_1 k \cos(\theta_1)(z_0 - d) + n_1 k \\ & \times \cos(\theta_1)(d - z)]\} p_i^u \end{aligned} \quad (35)$$

for $u = e, b$ and $i = 1, 2, 3$, where

$$\begin{aligned} p_1^e = & (1/2)\{[r_{TE} - r_{TM} \cos(\theta_1)]J_0[n_1 k \rho \sin(\theta_1)] \\ & + [r_{TE} + r_{TM} \cos(\theta_1)]J_2[n_1 k \rho \sin(\theta_1)]\}, \end{aligned} \quad (36a)$$

$$p_2^e = [r_{TE} + r_{TM} \cos(\theta_1)]J_2[n_1 k \rho \sin(\theta_1)], \quad (36b)$$

$$p_3^e = -ir_{TM} \sin(\theta_1)J_1[n_1 k \rho \sin(\theta_1)], \quad (36c)$$

$$\begin{aligned} p_1^b = & (-1/2)\{[r_{TM} - r_{TE} \cos(\theta_1)]J_0[n_1 k \rho \sin(\theta_1)] \\ & + [r_{TM} + r_{TE} \cos(\theta_1)]J_2[n_1 k \rho \sin(\theta_1)]\}, \end{aligned} \quad (36d)$$

$$p_2^b = -[r_{TM} + r_{TE} \cos(\theta_2)]J_2[n_1 k \rho \sin(\theta_1)], \quad (36e)$$

$$p_3^b = ir_{TE} \sin(\theta_1)J_1[n_1 k \rho \sin(\theta_1)]. \quad (36f)$$

The Fresnel reflection coefficients are

$$\begin{aligned} r_{TE} = & [\cos(\theta_1) - (n_2/n_1)\cos(\theta_2)] / [\cos(\theta_1) \\ & + (n_2/n_1)\cos(\theta_2)], \end{aligned} \quad (37a)$$

$$\begin{aligned} r_{TM} = & [(n_2/n_1)\cos(\theta_1) - \cos(\theta_2)] / [(n_2/n_1)\cos(\theta_1) \\ & + \cos(\theta_2)]. \end{aligned} \quad (37b)$$

Unlike the refracted beam, the reflected beam does not possess spherical aberration. If the plane wave incident upon the lens is linearly polarized in the y direction, the beam fields in the medium n_1 and those refracted or reflected by the plane interface at $z = d$ are given by Eqs. (13), with F_i^u given by Eqs. (26), (28), and (35) and p_i^u given by Eqs. (27), (29), and (36).

4. Beam Shape Coefficients in the Localized Model

A. General Considerations

In the GLMT formalism, shape coefficients g_l and h_l play a central role in the calculation of the near-zone and far-zone fields scattered by a spherical particle^{17,19} and the radiation trapping force on a spherical particle.^{16–18} The determination of these coefficients in specific situations, however, has posed somewhat of a practical problem. If one has an analytical formula for the beam fields (which we hereafter call the original beam), one could use Eqs. (5) to determine g_l and h_l by numerical integration. If the beam is an exact solution of Maxwell's equations, as is the case for a plane wave, the r dependence in Eqs. (5) cancels out and g_l and h_l are constants. But if the analytical formula for the original beam is not an exact solution of Maxwell's equations, as is the case for the freely diffracting focused Gaussian beam, a Davis first-order focused Gaussian beam, or a Davis–Barton symmetrized third-order or fifth-order focused Gaussian beam of Section 3, one has to evaluate Eqs. (5) at an arbitrarily chosen radial coordinate in order for the g_l and h_l thus obtained to be constants. The choice $r = a$, where a is the radius of the spherical particle upon which the beam impinges, has commonly been used.^{18,19} The $r = a$ evaluation procedure repairs the defect that the original beam was only an approximate solution of Maxwell's equations. By substituting the repaired g_l and h_l obtained from Eqs. (5) with $r = a$ into Eqs. (8), one can then reconstruct a beam that is both an exact solution of Maxwell's equations and a close approximation to the original beam. In principle, one must evaluate an infinite number of coefficients g_l and h_l to reconstruct the beam by using Eqs. (8). For scattering applications this is not necessary because, according to van de Hulst's localization principle, partial waves with $l \gg X$ effectively do not interact with a spherical particle whose size parameter is $X \equiv 2\pi a/\lambda$. The numerical integration required for determining g_l and h_l from the known original beam does not pose much of a computational burden if the particle involved is small and only a few partial waves, and thus only a few coefficients g_l and h_l , are required for convergence. But many partial waves contribute if

the particle involved is larger than $\sim 2 \mu\text{m}$ and the beam wavelength is in the visible region of the electromagnetic spectrum. Thus one must compute many integrals with rapidly varying integrands to determine g_l and h_l , a procedure that has proved to be both time consuming and inconvenient.

A second way to repair the defect that the original beam is only an approximate solution to Maxwell's equations is provided by the localized beam formalism. This formalism generates a second set of beam shape coefficients g_l and h_l from the known beam fields without integration. These coefficients are then used to reconstruct a beam that is both an exact solution to Maxwell's equations and a different close approximation to the original beam. These two ways to repair the original beam produce slightly different final beams that both closely approximate the original beam. Neither of the final two beams is intrinsically superior to the other because both are exact solutions to Maxwell's equations. What is true, though, is that both are superior to the original beam (such as the Davis–Barton fifth-order beam) because the original beam was not an exact solution to Maxwell's equations. Which of the two versions of the final beam one uses is a matter of computational convenience and personal taste. The localized final beam is used both here and in the research reported in Ref. 33.

For an original beam propagating in the z direction and linearly polarized in the x direction, the localized beam shape coefficients are obtained as follows: Assume that the analytical formula for functions F_i^u for the fields of the original beam is known for $i = 1, 2, 3$ and $u = e, b$. Both F_3^e and F_3^b are proportional to $\sin(\theta)$, as is demanded by Eqs. (8a), (8d), and (10c). In addition, let f_i^u be defined by

$$F_i^u \equiv f_i^u \exp(inkz) \quad (38)$$

for $i = 1, 2, 3$. Then e_r and b_r of Eqs. (1) may be written in terms of the quantities

$$f_r^e \equiv f_1^e + f_3^e \cos(\theta)/\sin(\theta), \quad (39a)$$

$$f_r^b \equiv f_1^b + f_3^b \cos(\theta)/\sin(\theta) \quad (39b)$$

as

$$e_r = \exp(inkz) f_r^e \sin(\theta) \cos(\phi), \quad (40a)$$

$$b_r = \exp(inkz) f_r^b \sin(\theta) \sin(\phi). \quad (40b)$$

The fact that f_3^e and f_3^b are proportional to $\sin(\theta)$ prevents f_r^e and f_r^b from diverging for $\theta = 0, \pi$. The shape coefficients of the localized beam are obtained from f_r^e and f_r^b by the prescription

$$g_l = f_r^e(nkr = l + 1/2, \theta = \pi/2) = f_1^e(nkr = l + 1/2, \theta = \pi/2), \quad (41a)$$

$$h_l = f_r^b(nkr = l + 1/2, \theta = \pi/2) = f_1^b(nkr = l + 1/2, \theta = \pi/2). \quad (41b)$$

The relation between g_l, h_l and f_r^e, f_r^b was derived in Refs. 20, 21, and 27. The relation between g_l, h_l, f_1^e and f_1^b is new and provides a more convenient prescription. From Eqs. (38) and (41), the analytical formula for F_1^e and F_1^b of the original beam generates shape coefficients g_l and h_l of the corresponding localized beam without requiring the angular integration of Eqs. (5).

The prescription for generating localized beams for the other three general on-axis beam geometries is similar. If the original beam propagates in the z direction and is linearly polarized in the y direction, the radial component of the fields may be written as

$$e_r = \exp(inkz) f_r^e \sin(\theta) \sin(\phi), \quad (42a)$$

$$b_r = -\exp(inkz) f_r^b \sin(\theta) \cos(\phi), \quad (42b)$$

with f_r^e and f_r^b given by Eqs. (39). If the beam propagates in the $-z$ direction and is linearly polarized in the x direction, one obtains

$$e_r = \exp(-inkz) f_r^e \sin(\theta) \cos(\phi), \quad (43a)$$

$$b_r = -\exp(-inkz) f_r^b \sin(\theta) \sin(\phi), \quad (43b)$$

with f_i^u now defined by

$$F_i^u \equiv f_i^u \exp(-inkz). \quad (44)$$

If the beam propagates in the $-z$ direction and is linearly polarized in the y direction, one obtains

$$e_r = \exp(-inkz) f_r^e \sin(\theta) \sin(\phi), \quad (45a)$$

$$b_r = \exp(-inkz) f_r^b \sin(\theta) \cos(\phi). \quad (45b)$$

For each of these four general on-axis geometries the localized beam-shape coefficients are obtained from f_r^e and f_r^b through Eqs. (41). As a simple check of this procedure, one can quickly see that the localized version of a plane wave is identical to the original plane wave because a plane wave is characterized by $f_r^e = f_r^b = 1$, leading by means of Eqs. (41) to $g_l = h_l = 1$, which are the beam shape coefficients of a plane wave.

B. Localized Gaussian Beams

The use of localized beams in light-scattering calculations has to date been almost solely confined to a moderately focused Gaussian beam. For tightly focused beams with relatively large s , the Davis–Barton fifth-order beam of Eqs. (24) becomes inaccurate because not enough powers of s are present to produce convergence. But at high s the localized focused Gaussian beam,²¹

$$g_l = h_l = D \exp(-inkz_0) \exp[-Ds^2(l + 1/2)^2], \quad (46)$$

which is generated from the Davis first-order beam with D evaluated at $z = 0$, is an exact solution of Maxwell's equations and is thus a valid beam description. Similarly, the Davis–Barton fifth-order beam in the Fraunhofer diffraction region upstream and

downstream from the focal waist becomes inaccurate for $\theta \gtrsim 45^\circ$ because again not enough terms of the beam expansion are present to produce convergence. This angular region in the diverging part of the beam is important in laser tweezer applications when the particle being held has a radius of a few micrometers because the geometrical rays associated with the diverging beam that is responsible for trapping are incident near the edge of the particle¹² and are often characterized by $\theta \gtrsim 45^\circ$. Again, the localized beam model, which is an exact solution of Maxwell's equations, is convergent in this important angular region and thus is a better candidate for the beam model than is the Davis–Barton fifth-order beam.

Reference 27 reports that a second version of the localized focused Gaussian beam propagating in the z direction and polarized in the x direction, called the modified localized beam, was generated by the shape coefficients

$$g_l = h_l = D \exp(-inkz_0) \exp[-Ds^2(l+2)(l-1)]. \quad (47)$$

For high partial waves, Eq. (47) becomes identical to Eq. (46). For low partial waves, Eq. (47) gives a better approximation to the original freely diffracting Gaussian beam or the Davis first-order beam than does the localized Gaussian beam, as can be seen in the following way: Consider a Gaussian beam whose focal waist is located at $z = z_0$. One can trace out the entire beam by considering only the xy plane (i.e., $\theta = \pi/2$) while varying z_0 . In particular, one can trace out the beam fields on the z axis by evaluating them at the origin while varying z_0 . At the origin, the Davis first-order beam of Eqs. (24) is

$$F_1^e = F_1^b = \exp(-inkz_0)/(1 - 2isz_0/w), \quad (48a)$$

$$F_2^e = F_2^b = F_3^e = F_3^b = 0. \quad (48b)$$

According to Eqs. (8), only partial wave $l = 1$ contributes to the localized and modified localized beams at the origin, giving

$$F_1^e = g_1, \quad (49a)$$

$$F_1^b = h_1, \quad (49b)$$

$$F_2^e = F_2^b = F_3^e = F_3^b = 0, \quad (49c)$$

while progressively more partial waves contribute as one moves out from the z axis in the xy plane. Whereas the localized Gaussian beam of Eqs. (6) at the origin is

$$F_1^e = F_1^b = \exp(-inkz_0) \exp\{-9s^2/[4(1 - 2isz_0/w)]\}/(1 - 2isz_0/w), \quad (50a)$$

$$F_2^e = F_2^b = F_3^e = F_3^b = 0, \quad (50b)$$

the modified localized beam of Eq. (47) agrees with Eqs. (48). As a result, whereas both the localized and the modified localized Gaussian beams closely match the falloff of the original Davis first-order

beam fields in the transverse direction, the modified beam more faithfully matches the falloff of the beam fields in the longitudinal direction. This distinction is significant for laser tweezer calculations because the optical trap is weakest in the z direction, and thus it is important to accurately model the z behavior of the fields.

One obtains the shape coefficients of the localized version of a plane wave focused and truncated by a high-NA lens by combining Eqs. (26), (27), and (38) and then using the prescription of Eqs. (41), arriving at

$$\begin{aligned} g_l = h_l = & -in_1 k F \int_0^\alpha \sin(\theta_1) d\theta_1 [\cos(\theta_1)]^{1/2} \\ & \times \exp[in_1 k(z - z_0) \cos(\theta_1)] (1/2) \{ [1 \\ & + \cos(\theta_1)] J_0[(l + 1/2) \sin(\theta_1)] + [1 \\ & - \cos(\theta_1)] J_2[(l + 1/2) \sin(\theta_1)] \}. \end{aligned} \quad (51)$$

On the basis of numerical computations not reported in detail here, the modified prescription appears not to provide an improved description of the fields of a plane wave focused and truncated by a lens.

5. Tightly Focused Localized Beams

A. Gaussian Beams

The Davis procedure for constructing a sequence of focused, approximately Gaussian beams that are increasingly better approximations to an exact solution of Maxwell's equations was devised with paraxial beams in mind, so the series solution in s is rapidly convergent. But, when a beam is tightly focused by a short-focal-length lens, the resultant focused beam is far from paraxial, and its shape becomes distorted with respect to that of a beam focused by a long-focal-length lens. In this section I compare both the original Gaussian beam and the focused and truncated beams of Section 3 with the associated beams reconstructed from the localized shape coefficients of Section 4. The comparison is made in the vicinity of the center of the focal waist, starting at the beam axis and going out either to the $1/e^2$ intensity point for the Gaussian beams or to the end of the Airy disk for the focused and truncated beams. The fields beyond the Airy disk are small and likely only weakly affect the trapping conditions of laser tweezers.

For an arbitrary on-axis beam propagating in a single medium as discussed in Section 3, one has $F_i^e = F_i^b = F_i$ for $i = 1, 2, 3$. Assuming that g_l and h_l are real, F_1 and F_2 in the focal plane are purely real and F_3 is purely imaginary. For this situation, the beam intensity in the focal plane reduces to

$$I_z = (nE_0^2/\mu_0 c) F_1(F_1 - F_2) \quad (52)$$

and is circularly symmetric no matter how tightly focused the beam is. The quantity $\mathbf{E}^* \cdot \mathbf{E}$ of Eq. (18)

Table 1. Actual $1/e^2$ Intensity Transverse Half-Width w_a of a Davis–Barton Fifth-Order Focused Gaussian Beam (D5) and a Localized Focused Gaussian Beam (L) at the Center of the Focal Waist As a Function of Intended Half-Width w_i for $\lambda = 1.06 \mu\text{m}$ and $n_1 = 1.50$

w_i (μm)	s_i	w_a^{D5} (μm)	w_a^{L} (μm)
5.00	0.0225	5.00	5.00
4.00	0.0281	4.00	4.00
3.00	0.0375	3.00	3.00
2.00	0.0562	2.00	2.01
1.00	0.1125	1.00	1.02
0.80	0.1406	0.81	0.82
0.60	0.1874	0.61	0.63
0.40	0.2812	0.42	0.44
0.20	0.5623	0.23	0.29

in the focal plane of an arbitrary on-axis beam propagating in a single medium reduces to

$$\mathbf{E}^* \cdot \mathbf{E} = E_0^2 \{ [F_1^2 + |F_3|^2 + (F_1 - F_2)^2]/2 + \cos(2\phi) \times (|F_3|^2 - F_2^2 + 2F_1F_2)/2 \}, \quad (53)$$

which is nearly circularly symmetric for a mildly focused beam with $s \ll 1$ such that $|F_3| \ll F_1$ and $F_2 \ll F_1$ but is noticeably elliptical for a tightly focused beam with larger s and nonnegligible F_2 and $|F_3|$. If the width of a Gaussian beam incident upon a lens is much smaller than the lens aperture, the transmitted beam is modeled by a focused Gaussian beam. For the fifth-order Davis–Barton beam approximation, the intensity in the focal plane of Eq. (52) is

$$I_z = (nE_0^2/\mu_0 c) \exp(-2\rho^2/w^2) [1 + s^2(4\rho^2/w^2 - 2\rho^4/w^4) + s^4(15\rho^4/w^4 + 4\rho^6/w^6 + 2\rho^8/w^8) + O(s^6)]. \quad (54)$$

Even for tight focusing and relatively large s , the deviation of the beam profile from a Gaussian shape in the strongest part of the beam is numerically found to be small for both the Davis–Barton beam of Eqs. (24) and the localized focused Gaussian beam of Eqs. (8a)–(8f) and (47). The greatest distortion of the beam shape is an increase in the actual width of the beam with respect to the intended width w that appears in the beam formulas. Typical Gaussian beam parameters for laser tweezer modeling are $\lambda = 1.06 \mu\text{m}$ and $n_1 = 1.50$. For these parameters, the Davis–Barton fifth-order beam intensity was calculated from Eqs. (24) and (52) and the localized Gaussian beam was reconstructed as follows: In Eqs. (8) the sum over partial waves is computed as in a traditional Mie scattering program. The beam shape coefficients that appear in Eqs. (8) are given by Eq. (47), and the spherical Bessel functions are computed in double precision by use of upward recursion up to the maximum partial wave $l_{\text{max}} = 1 + nkr + 4.3(nkr)^{1/3}$. The results are substituted into Eqs. (10), and then those results are substituted into Eq. (52). The actual $1/e^2$ intensity half-width w_a for both beams is shown in Table 1 to correspond to a given intended width w_i . The actual width is al-

ways somewhat larger than the intended width, but the difference becomes vanishingly small for $w_i \gtrsim 1.0 \mu\text{m}$ or $s \lesssim 0.1$. Thus, when a tightly focused Gaussian beam of a given actual width is desired, the intended width used as input in a GLMT calculation of the trapping force should be chosen correspondingly smaller. The fact that for tight focusing the actual localized beam width is larger than that of the Davis–Barton fifth-order beam approximation for a given intended width does not imply that the localized beam is less accurate than the Davis–Barton beam. The larger actual width appears to be the price that one has to pay to force the beam to be constrained in a region substantially smaller than the wavelength of light and yet be an exact solution of Maxwell's equations.

In the focal plane of a fifth-order Davis–Barton focused Gaussian beam, Eq. (53) becomes

$$\mathbf{E}^* \cdot \mathbf{E} = E_0^2 \exp(-2\rho^2/w^2) [1 + s^2(6\rho^2/w^2 - 2\rho^4/w^4) + 4s^2 \cos(2\phi)\rho^2/w^2 + O(s^4)]. \quad (55)$$

The analogous expression used in Ref. 10 contains the z component of the Davis first-order field but omits the x component of the Davis–Barton third-order field, which is of the same size. The widths of $\mathbf{E}^* \cdot \mathbf{E}$ for this beam in the x and y directions in the focal plane are

$$w_x^{\text{actual}} = 2 \left[\int_0^\infty x^2 \mathbf{E}^*(\phi = 0) \cdot \mathbf{E}(\phi = 0) dx \right]^{1/2} = w [1 + 7s^2/4 + O(s^4)], \quad (56a)$$

$$w_y^{\text{actual}} = 2 \left[\int_0^\infty y^2 \mathbf{E}^*(\phi = \pi/2) \cdot \mathbf{E}(\phi = \pi/2) dy \right]^{1/2} = w [1 - s^2/4 + O(s^4)]. \quad (56b)$$

The actual width increases from the intended width in the x direction, whereas it decreases in the y direction. The resultant ellipticity of $\mathbf{E}^* \cdot \mathbf{E}$ for a tightly focused Gaussian beam is apparent in Fig. 9 of Ref. 10. From computed results not reported in detail here, numerical reconstruction of a localized focused Gaussian beam for $\lambda = 1.06 \mu\text{m}$, $n_1 = 1.50$, and various values of w_i showed that the $1/e^2$ values $\mathbf{E}^* \cdot \mathbf{E}$ in the x and y directions were virtually the same as those found for a fifth-order Davis–Barton focused Gaussian beam.

B. Plane Wave Focused by a High-NA Lens

When a plane wave is focused by a high-NA lens (rather than by a long-focal-length lens) and is prop-

Table 2. Focal Plane Airy Disk Radius ρ_{Airy} in Medium n_1 of the Original and Localized Versions of a Plane Wave Focused by a Lens As a Function of Maximum Convergence Angle α of the Lens for $\lambda = 1.06 \mu\text{m}$ and $n_1 = 1.50$

α (deg)	NA	ρ_{Airy} (μm)		
		Original Beam of Eqs. (26) and (27)	Localized Beam	Eq. (57)
5	0.131	5.0	5.0	5.00
10	0.261	2.51	2.52	2.51
20	0.513	1.27	1.29	1.27
30	0.750	0.85, 0.88	0.89, 0.92	0.87
40	0.964	0.66, 0.70	0.70, 0.74	0.68
50	1.149	0.54, 0.60	0.60, 0.65	0.57
60	1.299	0.46, 0.54	0.54, 0.60	0.50

agating in a single medium, an interesting change occurs in the focal plane fields. The radius of the Airy disk in the focal plane for both the angular-spectrum-of-plane-waves original beam of Eqs. (26) and (27) and the reconstructed localized version of this beam was numerically computed as a function of the maximum convergence angle of the lens, α , in Eq. (25) for $\lambda = 1.06 \mu\text{m}$ and $n_1 = 1.50$. The computed Airy disk radius of these beams is given in Table 2.

The largest value of the lens convergence angle considered here is $\alpha = 60^\circ$, because for $\alpha > 62.5^\circ$ light incident upon the interface between the $n_1 = 1.50$ and $n_2 = 1.33$ media is totally internally reflected rather than refracted. It was found that, for $\alpha \leq 30^\circ$, the Airy disk radius for both the original beam and the reconstructed localized beam is well fitted by

$$\rho_{\text{Airy}} = 0.617\lambda/\text{NA}. \quad (57)$$

But, for $\alpha \geq 30^\circ$, the focusing of the beam by the lens is sufficiently tight and F_2 becomes sufficiently large that the first zero of F_1 and $F_1 - F_2$ in Eq. (52) differ substantially from each other. This results in a pair of closely spaced intensity zeros, the smaller of which corresponds to the first zero of $F_1 - F_2$ and the larger corresponds to the first zero of F_1 . The locations of both of these zeros are given in Table 2 for $\alpha \geq 30^\circ$. The beam intensity between the two zeros remains small, giving the visual appearance of an anomalously wide first relative minimum of the intensity. The average of the first zero of F_1 and $F_1 - F_2$ for $\alpha \geq 30^\circ$ for the original beam is still well fitted by Eq. (57), whereas for the reconstructed localized beam the Airy disk is somewhat wider, as was found to be the case for a focused Gaussian beam. In addition, by Taylor series expanding Eqs. (26) and (27) in powers of $\sin(\theta_1)$ and integrating⁴⁸ over the angle θ_1 term by term, then substituting the result into Eq. (52) and integrating⁴⁹ over the xy plane, it was found that the power of the focused plane wave evaluated at the center of the focal waist is

$$P = (E_0^2/\mu_0 c)\pi F^2 \sin^2(\alpha) + O[\sin^{10}(\alpha)] \quad (58)$$

and is well approximated by only the $\sin^2(\alpha)$ term.

Although a beam focused by a high-NA lens and

Table 3. Focal Plane Airy Disk Radius ρ_{Airy} Along the x and y Axes of the Original and Localized Versions of a Plane Wave Focused by a Lens and Reflected by a Flat Interface As a Function of Maximum Convergence Angle α of the Lens for $\lambda = 1.06 \mu\text{m}$, $n_1 = 1.50$, and $n_2 = 1.33$

α (deg)	NA	ρ_{Airy}^x (μm)		ρ_{Airy}^y (μm)	
		Original		Original	
		Beam of Eqs. (35) and (36)	Localized Beam	Beam of Eqs. (35) and (36)	Localized Beam
5	0.131	5.03	5.03	4.97	4.97
10	0.261	2.55	2.55	2.49	2.49
20	0.513	1.32	1.35	1.22	1.25
30	0.750	0.96	1.00	0.79	0.83
40	0.964	0.83	0.86	0.57	0.60
50	1.149	0.77	0.80	0.44	0.48
60	1.299	0.71	0.75	0.30	0.32

propagating in a single medium has a circularly symmetric intensity, when it is normally incident upon a flat interface placed before the intended focal waist the shape of the intensity profile of the reflected and refracted beams becomes elliptical. This is so because $F_i^e \neq F_i^b$ for the reflected and refracted beams, $g_l \neq h_l$ in the localized beam reconstruction, and Eq. (17) rather than Eq. (52) must be used for the intensity. Numerical computation for $\lambda = 1.06 \mu\text{m}$, $n_1 = 1.50$, and $n_2 = 1.33$ and various values of α in the paraxial focal plane of a beam focused by a lens and then transmitted through a flat interface shows that for both the original transmitted beam of Eqs. (28) and (29) and the reconstructed localized transmitted beam of Eqs. (8), (10), and (41) the ellipticity of the transmitted intensity profile is small, even for tight focusing. This small ellipticity should have only minor consequences for laser tweezer applications.

But the ellipticity of the intensity profile of the reflected beam can become surprisingly large. Table 3 gives the Airy disk radius in the x and y directions in the focal plane for both the original reflected beam of Eqs. (35) and (36) and the reconstructed localized reflected beam. For low NA, the reflected beam profile is nearly circularly symmetric, whereas for a high-NA lens the predicted aspect ratio of the beam profile grows to more than 2:1 for both the original and the reconstructed localized beams. The difference in the reflected Airy disk widths along the x and y axes is due to the fact that $F_1^b(\rho = 0)$ is smaller than $F_1^e(\rho = 0)$ and has its first zero for smaller ρ . This effect in turn is caused by the constructive interference of the various plane waves in the angular spectrum in the x direction and the destructive interference in the y direction, owing to modulation by different Fresnel reflection coefficients. As was found to be the case for both a focused Gaussian beam and a plane wave focused by a lens and propagating in a single medium, the actual width of the localized reflected beam is somewhat wider than that of the original reflected beam.

6. Conclusions

The two principal results of this paper concern (i) the appropriateness of using localized beams in GLMT calculations that involve tight beam confinement and (ii) a practical prescription for compensating for one of the idiosyncrasies of tightly confined beams. It was previously demonstrated that a reconstructed on-axis localized Gaussian beam propagating in the z direction and linearly polarized in the x direction provides a good approximation to the original on-axis focused Gaussian beam when the beam is mildly focused and the resultant beam confinement parameter s is small. In this paper it has been shown that localized beams accurately model original beams whose shape is Gaussian or otherwise and that are tightly confined, e.g., a plane wave truncated and focused by a high-NA lens and then aberrated by transmission through a flat interface. The prescription for generating localized beams to polarization in the y direction and propagation in the $-z$ direction was also generalized to describe circularly polarized beams and reflected beams. For all the beam types tested here, the localized version of the original beam was found to be somewhat less tightly focused than was the original beam from which it was generated. As a result, when a localized beam of a given focal width is desired, the intended beam width used as input in the GLMT calculation should be correspondingly smaller. In summary, localized beams have been demonstrated in this paper to provide a useful and accurate description of the types of beam commonly encountered in on-axis laser tweezers applications.

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